Topological aspects of quantum spin Hall effect in graphene: Z_2 topological order and spin Chern number

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(Dated: July 19, 2006)

For generic time-reversal invariant systems with spin-orbit couplings, we clarify a close relationship between the Z_2 topological order and the spin Chern number proposed by Kane and Mele and by Sheng *et al.*, respectively, in the quantum spin Hall effect. It turns out that a global gauge transformation connects different spin Chern numbers (even integers) modulo 4, which implies that the spin Chern number and the Z_2 topological order yield the same classification. We present a method of computing spin Chern numbers and demonstrate it in single and double plane of graphene.

PACS numbers: 73.43.-f, 72.25.Hg, 73.61.Wp, 85.75.-d

Topological orders [1, 2] play a crucial role in the classification of various phases in low dimensional systems. The integer quantum Hall effect (IQHE) is one of the most typical examples [3, 4], in which the quantized Hall conductance is given by a topological invariant, Chern number, due to the Berry phase [5] induced in the Brillouin zone [6]. Such a topological feature should be more fundamental, since it has a close relationship with the parity anomaly of Dirac fermions [7, 8, 9].

Recently, the spin Hall effect [10, 11, 12, 13] has been attracting much current interest as a new device of so-called spintronics. In particular, Kane and Mele [14, 15] have found a new class of insulator showing the quantum spin Hall (QSH) effect [16, 17, 18] which should be realized in graphene with spin-orbit couplings. They have pointed out [15] that the QSH state can be specified by a Z_2 topological order which is inherent in time-reversal ($\mathcal{T}$) invariant systems. This study is of fundamental importance, since the Z_2 order is involved with the Z_2 anomaly of Majorana fermions [19, 20].

On the other hand, Sheng *et al.* [21] have recently computed the spin Hall conductance by imposing spin-dependent twisted boundary condition, generalizing the idea of Niu *et al.* [2, 22]. They have shown that it is given by a Chern number which is referred to as a spin Chern number below. This seems very natural, since the QSH effect is a spin-related version of IQHE. The spin Chern number for graphene computed by Sheng *et al.* indeed has a good correspondence with the classification by Z_2.

However, the Chern number is specified by the set of integers Z, not by Z_2. Although the studies by Sheng *et al.* [21] suggest a close relationship between two topological orders, natural questions arise: How does the concept Z_2 enter into the classification by Chern numbers, or otherwise, does the spin Chern number carry additional information?

In this letter, we clarify the relationship for generic $\mathcal{T}$ invariant systems. We show that while two sectors in the Z_2 classification are separated by topological changes due to *bulk gap-closing phenomena*, each of these sectors is further divided into many sectors by *boundary-induced topological changes* in the spin Chern number classification. The latter is an artifact which is due to calculations in finite size systems with broken translational invariance. Therefore, the different spin Chern numbers in each sector of Z_2 describe the same topologically ordered states of the bulk.

Consider generic electron systems on a lattice with $\mathcal{T}$ symmetry, described by the Hamiltonian H. Denote the electron creation operator at jth site as $c_j^\dagger = (c_{\uparrow j}^\dagger, c_{\downarrow j}^\dagger)$. Then, $\mathcal{T}$ transformation is defined by $c_j \to \mathcal{T} c_j$ with $\mathcal{T} \equiv i\sigma^2 K$, where the Pauli matrix σ^2 operates the spin space and K stands for the complex conjugation operator. Let $\mathcal{H}(k)$ be the Fourier-transformed Hamiltonian defined by $H = \sum_k c^\dagger(k)\mathcal{H}(k)c(k)$ and let $|n(k)\rangle$ be an eigenstate of $\mathcal{H}(k)$. Assume that the ground state is composed of an M-dimensional multiplet of degenerate single particle states which is a generalized non-interacting Fermi sea [2]. Kane and Mele [15] have found that the $\mathcal{T}$ invariant systems have two kinds of important states belonging to "even" subspace and "odd" subspace: The states in the even subspace have the property that $|n(k)\rangle$ and $\mathcal{T}|n(k)\rangle$ are identical, which occurs when $\mathcal{T}\mathcal{H}(k)\mathcal{T}^{-1} = \mathcal{H}(k)$. By definition, the states at $k = 0$ always belong to this subspace. The odd subspace has the property that the multiplet $|n(k)\rangle$ are orthogonal to the multiplet $\mathcal{T}|n(k)\rangle$. These special subspaces can be detected by the pfaffian $p_{\rm KM}(k) \equiv \mathrm{pf}\ \langle n(k)|\mathcal{T}|m(k)\rangle$. Namely, $p_{\rm KM}(k) = 1$ in the even subspace and 0 in the odd subspace. Kane and Mele have claimed that the number of zeros of $p_{\rm KM}(k)$ which always appear as $\mathcal{T}$ pairs $\pm k^*$ with opposite vorticities is a topological invariant for $\mathcal{T}$ invariant systems. Specifically, if the number of zeros in half the Brillouin zone is 1 (0) mod 2, the ground state is in the QSH (insulating) phase.

We now turn to the spin Chern number proposed by

Sheng *et al.* [21]. According to their formulation, we impose spin-dependent (-independent) twisted boundary condition along 1(2)-direction

$$c_{j+L_1\hat{1}} = e^{i\theta_1\sigma^3}c_j, \quad c_{j+L_2\hat{2}} = e^{i\theta_2}c_j, \tag{1}$$

where a set of integers $j \equiv (j_1, j_2)$ specifies the site and $\hat{1}$ and $\hat{2}$ stand for the unit vectors in 1- and 2-directions, respectively. Let $\mathcal{H}(\theta)$ denote the twisted Hamiltonian and let $|n(\theta)\rangle$ be corresponding eigenstate. It follows from Eq. (1) that $\mathcal{T}$ transformation induces $\mathcal{T}\mathcal{H}(\theta_1,\theta_2)\mathcal{T}^{-1} = \mathcal{H}(\theta_1,-\theta_2)$ and therefore we can always choose $|n(\theta_1,-\theta_2)\rangle = \mathcal{T}|n(\theta_1,\theta_2)\rangle$ except for $\theta_2 = 0$. The states on the *line* $\theta_2 = 0$ belong to the even subspace. Below, the torus spanned by θ is referred to as twist space. The boundary condition (1) enables us to define the spin Chern number, but the cost we have to pay is the broken translational invariance. In other words, we slightly break $\mathcal{T}$ invariance at the boundary, which leads to nontrivial spin Chern numbers. The average over the twist angles recovers $\mathcal{T}$ invariance.

Let us define a pfaffian for the present twisted system as a function of the twist angles:

$$p(\theta) \equiv \text{pf } \langle n(\theta)|\mathcal{T}|m(\theta)\rangle, \quad n, m = 1, \cdots, M, \tag{2}$$

where M is a number of one particle states below the Fermi energy with the gap opening condition. Since the line $\theta_2 = 0$ belongs to the even subspace, the zeros of the pfaffian in the $\theta_2 > 0$ or < 0 twist space can move only among the same half twist space keeping their vorticities, and never cross the $\theta_2 = 0$ line. Therefore, one $\mathcal{T}$ pair of zeros are never annihilated, like those of the KM pfaffian $p_{\rm KM}(k)$. Furthermore, the two zeros in the same half twist space are never annihilated unless they have the opposite vorticity. This is a crucial difference between the KM pfaffian and the twist pfaffian. The number of zeros in the twist pfaffian should be classified by even integers (half of them, by Z).

Are these pfaffians topologically different quantities? The answer is no. To show this, let us consider a global gauge transformation $c_j \to g(\varphi)c_j$, where

$$g(\varphi) \equiv e^{i\sigma^2\varphi} = \cos\varphi + i\sigma^2 \sin\varphi. \tag{3}$$

This transformation replaces the the Pauli matrices in the spin-orbit couplings into $g^{\rm t}(\varphi)\boldsymbol{\sigma}g(\varphi) = (\cos 2\varphi\,\sigma^1 - \sin 2\varphi\,\sigma^3, \sigma^2, \cos 2\varphi\,\sigma^3 + \sin 2\varphi\,\sigma^1)$. On the other hand, since Eq. (3) is an orthogonal transformation, one-parameter family of transformed Hamiltonian, denoted by H^φ or $\mathcal{H}^\varphi(\theta)$ below, is equivalent. The pfaffian (2) is also invariant. Therefore, when we are interested in the bulk properties, we can deal with any Hamiltonian H^φ.

So far we have discussed the bulk properties. However, if we consider finite periodic systems like Eq. (1), a family of the Hamiltonian H^φ behaves as different models. It follows from Eq. (1) that the gauge transformation (3) is commutative with $e^{i\theta_2}$, but *not* with $e^{i\theta_1\sigma^3}$. This tells us that spin-dependent twisted boundary condition is not invariant under the gauge transformation (3), and breaks the gauge-equivalence of the Hamiltonian H^φ which the bulk systems should have.

To understand this, the following alternative consideration may be useful: If we want to study bulk properties of $\mathcal{T}$ invariant systems, we can start with any of H^φ. For one H^φ with φ fixed, let us impose the twisted boundary condition (1). After that, we can make a gauge transformation (3) back to H^0. Then, we can deal with the original Hamiltonian H^0, but with a gauge-dependent twisted boundary condition for x-direction;

$$c_{j+L_1\hat{1}} = e^{i\theta_1(\cos 2\varphi\sigma^3 - \sin 2\varphi\sigma^1)}c_j. \tag{4}$$

Namely, the gauge equivalence is broken only by the boundary condition in 1-direction. Now, imagine a situation that at $\varphi = 0$ the pfaffian (2) has one $\mathcal{T}$ pair of zeros. We denote them as $(\theta_1^*, \pm\theta_2^*)$ with vorticity $\pm m$. Let us change φ smoothly from 0 to $\pi/2$. Then, it follows from Eq. (4) that at $\varphi = \pi/2$ the coordinate of the torus is changed from (θ_1,θ_2) into $(-\theta_1,\theta_2)$ and therefore, we find the zeros at $(-\theta_1^*, \pm\theta_2^*)$ with vorticity $\mp m$. We thus have a mapping $(\theta_1^*, \pm\theta_2^*) \to (-\theta_1^*, \mp\theta_2^*)$ for $\varphi = 0 \to \pi/2$. Namely, the zero in the $\theta_2 > 0$ (< 0) space moves into the $\theta_2 < 0$ (> 0) space, and thus the zeros can move in the whole twist space like those of the KM pfaffian. During the mapping, there should occur a topological change, but it is attributed to the boundary, i.e, an artifact of broken translational invariance, and half of the zeros of twist pfaffian should be also classified by Z_2, by taking into account the gauge transformation (3).

Using this pfaffian, we next show that its zeros can be detectable by computing the spin Chern number which seems much easier to perform than searching them directly. The spin Chern number [21] is defined by $c_{\rm s} = \frac{1}{2\pi i}\int d^2\theta F_{12}(\theta)$, where $F_{12}(\theta) \equiv \partial_1 A_2(\theta) - \partial_2 A_1(\theta)$ is the field strength due to the U(1) part of the (non-Abelian) Berry potential [2], $A_\mu(\theta) \equiv {\rm tr}\langle n(\theta)|\partial_\mu|m(\theta)\rangle$ with $\partial_\mu = \partial/\partial\theta_\mu$. First, we will show the relationship between the zeros of the twist pfaffian and the spin Chern number $c_{\rm s}$. For the time being, we fix φ. The degenerate ground state as the M-dimensional multiplet has a local U(M) gauge degree of freedom, $|n(\theta)\rangle \to \sum_m |m(\theta)\rangle V_{mn}(\theta)$, where $V(\theta)$ is a unitary matrix [2]. Let us denote $V(\theta) = e^{i\alpha(\theta)/M}\tilde{V}(\theta)$, where $\det\tilde{V}(k) = 1$. This transformation induces $A_\mu(\theta) \to A_\mu(\theta) + i\partial_\mu\alpha(\theta)$ to the Berry potential. If one can make gauge-fixing globally over the whole twist space, the Chern number is proved to be zero. Only if the global gauge-fixing is impossible, the Chern number can be nonzero.

Among various kinds of gauge-fixing, we can use the gauge that $p(\theta)$ *is real positive*, because $p(\theta) \to p(\theta)\det V(\theta) = p(\theta)e^{i\alpha(\theta)}$. This rule can fix the gauge of the Berry potential except for $p(\theta) = 0$. Therefore,

nontrivial spin Chern number is due to an obstruction to the smooth gauge-fixing by the twist pfaffian. This correspondence also proves that *the spin Chern number is an even integer*, since the pfaffian (2) always has $\mathcal{T}$ pair zeros, and since $F_{12}(\theta_1,-\theta_2)=F_{12}(\theta_1,\theta_2)$.

Let us now change φ. At $\varphi=0$, we obtain a certain integral $c_{\rm s}$. Remember that at $\varphi=\pi/2$, the coordinate of the torus is changed into $(-\theta_1,\theta_2)$. Therefore, we have a mapping $c_{\rm s}\to -c_{\rm s}$ for $(\theta_1,\theta_2)\to(-\theta_1,\theta_2)$. As in the case of the pfaffian (2), we expect topological changes during the mapping. However, as stressed, these changes are accompanied by *no gap-closing in the bulk spectrum*, just induced by the symmetry breaking *boundary* term which is an artifact to define the Chern numbers. Therefore, the states with $\pm c_{\rm s}$ should belong to an equivalent topological sector. Since the minimum nonzero spin Chern number is 2, we expect $c_{\rm s}$ mod 4 (if we define the spin Chern number in half the twist space, mod 2) classifies the topological sectors.

So far we have discussed the Z_2 characteristics of the spin Chern number $c_{\rm s}$. We next present several examples. To this end, we employ an efficient method of computing Chern numbers proposed in Ref. [23]. We first discretize the twist space $[0,2\pi]\otimes[0,2\pi]$ into a square lattice such that $\theta_\mu=2\pi j_\mu/N_\mu$, where $j_\mu=1,\cdots,N_\mu$ [24]. We denote the sites on this lattice as θ_ℓ with $\ell=1,2,\cdots,N_1N_2$. We next define a U(1) link variable associated with the ground state multiplet of the dimension M,

$$U_\mu(\theta_\ell)=|\det\boldsymbol{U}_\mu(\theta_\ell)|^{-1}\det\boldsymbol{U}_\mu(\theta_\ell),$$

where $\boldsymbol{U}_\mu(\theta_\ell)_{mn}=\langle m(\theta_\ell)|n(\theta_\ell+\hat\mu)\rangle$ with $n,m=1,\cdots,M$ denotes the (non-Abelian) Berry link variable. Here, $\hat\mu$ is the vector in μ direction with $|\hat\mu|=2\pi/N_\mu$. Next define the lattice field strength,

$$F_{12}(\theta_\ell)=\ln U_1(\theta_\ell)U_2(\theta_\ell+\hat1)U_1^{-1}(\theta_\ell+\hat2)U_2^{-1}(\theta_\ell),$$

where we choose the branch of the logarithm as $|F_{12}(\theta_\ell)|<\pi$. Finally, manifestly *gauge invariant* lattice Chern number is obtained:

$$c_{\rm s}=\frac{1}{2\pi i}\sum_\ell F_{12}(\theta_\ell). \tag{5}$$

As shown in [23], the spin Chern number thus defined is strictly *integral*. To see this, let us introduce a lattice gauge potential $A_\mu(\theta_\ell)=\ln U_\mu(\theta_\ell)$ which is also defined in $|A_\mu(\theta_\ell)|<\pi$. Note that this field is periodic, $A_\mu(\theta_\ell+N_\mu)=A_\mu(\theta_\ell)$. Then, we readily find

$$F_{12}(\theta_\ell)=\Delta_1A_2(\theta_\ell)-\Delta_2A_1(\theta_\ell)+2\pi i n_{12}(\theta_\ell), \tag{6}$$

where Δ_μ stands for the difference operator and $n_{12}(\theta_\ell)$ is a local *integral* field which is referred to as n-field. Finally, we reach $c_{\rm s}=\sum_\ell n_{12}(\theta_\ell)$. This completes the proof that the spin Chern number is integral. While the n-field depends on a gauge we adopt, the sum is invariant. For the $\mathcal{T}$ invariant systems, *the pfaffian (2) is very useful for the gauge-fixing* also for the lattice computation. In the continuum theory, we have stressed that the zeros of the pfaffian play a central role in the Z_2 classification. Since such zeros occur at several specific points in the twist space, it is very hard to search them numerically.

Contrary to this feature in the continuum approach, we can detect the zeros in the lattice approach as follows: Suppose that we obtain an exact Chern number using Eq. (5) with sufficiently large N_μ. Since the lattice Chern number is topological (integral), which implies that even if we slightly change the lattice (e.g, change the lattice size or infinitesimally shift the lattice), the Chern number remains unchanged. Next, let us compute the n-field in the gauge that *the pfaffian is real positive*. If the zeros of the pfaffian happen to locate on sites of the present lattice, we cannot make gauge-fixing. Even in such cases, we can always avoid the zeros of the pfaffian by redefining the lattice with the spin Chern number kept unchanged. Thus we can always compute the well-defined n-field configuration. If the Chern number is nonzero, there exist nonzero n-field somewhere in the twist space. These nonzero n-field occur in general near the zeros of the pfaffian: Thus, without searching zeros of pfaffian in the continuum twist space, we can observe *the trace of such zeros as nonzero n-fields*.

Now let us study a graphene model with spin-orbit couplings [14, 15, 21];

$$\begin{aligned}H=&-t\sum_{\langle i,j\rangle}c_i^\dagger c_j+\frac{2i}{\sqrt3}V_{\rm so}\sum_{\langle\langle i,j\rangle\rangle}c_i^\dagger\boldsymbol{\sigma}\cdot(\boldsymbol{d}_{kj}\times\boldsymbol{d}_{ik})\,c_j\\&+iV_{\rm R}\sum_{\langle i,j\rangle}c_i^\dagger\,(\boldsymbol{\sigma}\times\boldsymbol{d}_{ij})^3\,c_j+v_{\rm s}\sum_j{\rm sgn}j\;c_j^\dagger c_j,\end{aligned} \tag{7}$$

where $c_j^\dagger=(c_{\uparrow j}^\dagger,c_{\downarrow j}^\dagger)$ is the electron creation operator at site j on the honeycomb lattice, sgn$j$ denotes 1 (-1) if j belongs to the A (B) sublattice, and $\boldsymbol{d}_{ij}$ stands for the vector from j to i sites. The first term is the nearest neighbor hopping, the second term is the s_z-conserving next-nearest neighbor spin-orbit coupling, whereas the third term is the Rashba spin-orbit coupling, and final term is a on-site staggered potential. Analyzing the KM pfaffian, Kane and Mele [14] have derived the phase diagram: It is in the QSH phase for $|6\sqrt3V_{\rm so}-v_{\rm s}|>\sqrt{v_{\rm s}^2+9V_{\rm R}^2}$ and in the insulating phase otherwise. Sheng *et. al.* [21] have computed the spin Chern number $c_{\rm s}=2$ in the QSH phase and 0 in the insulating phase.

For numerical computations, it is convenient to use the momentum k_2 [21, 25] instead of θ_2 because of the translational invariance along this direction even with the boundary condition (1). First, we show the spectrum in Fig. 1 at $\theta_1=0$ as a function of k_2. The left belongs to the QSH phase with $c_{\rm s}=2$, whereas the right to the insulating phase with $c_{\rm s}=0$. This topological change is

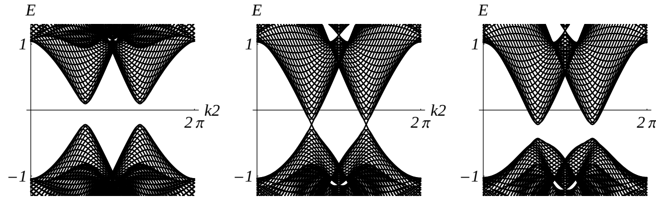

FIG. 1: Spectrum for $\theta_1 = 0$ as a function of k_2. Parameters used are $V_{\rm so} = 0.1t$, $v_{\rm s} = 0.3t$, and $V_{\rm R} = 0.1t$ (left), $V_{\rm R} = 0.225207t$ (middle), and $V_{\rm R} = 0.3t$ (right).

due to the gap-closing in the *bulk* spectrum, as shown in the middle in Fig. 1. Therefore, the phase with $c_{\rm s} = 2$ is topologically distinguishable from the phase with $c_{\rm s} = 0$.

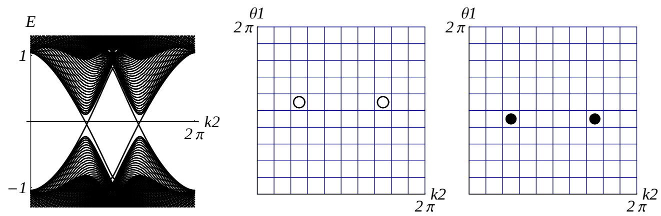

FIG. 2: Left: Spectrum for nonzero $\varphi = \pi/4$ as a function of k_2 at $\theta_1 = \pi/2$. Other parameters are the same as those of the left in Fig. 1. Right two: the n-field configuration corresponding to the left in Fig. 1. The left (right) is at $\varphi = 0$ ($\pi/2$). The white (black) circle denotes $n = 1$ (-1), while the blank means $n = 0$. We used the meshes $N_1 = N_2 = 10$.

Contrary to this, how about the phases with $c_{\rm s} = \pm 2$? As we have mentioned, the phase with $c_{\rm s}$ changes into $-c_{\rm s}$ when we vary φ from 0 to $\pi/2$. In this process, *boundary*-induced topological changes must occur. We show in Fig. 2 the spectrum cut at $\theta_1 = \pi/2$ for $\varphi = \pi/4$. We indeed observe a gap-closing at finite θ_1, and the spin Chern number $c_{\rm s} = 2$ for $0 \le \varphi < \pi/4$ is changed into $c_{\rm s} = -2$ for $\pi/4 < \varphi \le \pi/2$. As stressed, this change is attributed to the boundary (edge states in Fig. 2), not to the bulk, and we conclude that the phase $c_{\rm s} = \pm 2$ is classified as the same QSH phase. These spin Chern numbers $c_{\rm s} = \pm 2$ are well visible by the n-field. In Fig. 2, we also show the n-field for $\varphi = 0$ and $\pi/2$ cases in the QSH phase. The points of nonzero n-field is closely related with the positions of the pfaffian zeros. We also note that in Eq. (5) net contributions to the nonzero Chern number is just from two points.

Next, let us study a bilayer graphene. Suppose that we have two decoupled sheets of graphene described by H^{φ_i} with $i = 1, 2$ whose lattices include A, B sites and $\tilde{A}$, $\tilde{B}$ sites, respectively. For simplicity, we take into account only the interlayer coupling γ_1 between $\tilde{A}$ and B [26]: $V_{12} = \gamma_1 \sum_j c^\dagger_{1\tilde{A},j} c_{2B,j} + $ h.c., where $i = 1, 2$ in $c_{i,j}$ indicate the ith sheet. Now make the gauge transformation (3) separately for each sheet to obtain the same H^0 as Eq. (7). Then, we have identical bilayer system $H^0 \otimes H^0$ coupled by $V_{12} = \gamma_1 \sum_j c^\dagger_{1\tilde{A},j} g(\varphi_1) g^{\rm t}(\varphi_2) c_{2B,j+}$h.c. with two independent boundary conditions $c_{i,j+L_1\hat{1}} = e^{i\theta_1(\cos 2\varphi_i \sigma^3 + \sin 2\varphi_i \sigma^1)} c_{i,j}$.

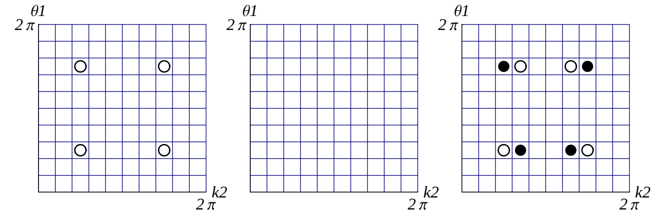

FIG. 3: The n-field configuration for $\gamma_1 = 0.1t$. Other parameters are same as those of the left in Fig. 1. Left: $\varphi_1 = 0$ and $\varphi_2 = 0$. Middle: $\varphi_1 = \pi/2$ and $\varphi_2 = 0$. Right: $\varphi_1 = \pi/4$ and $\varphi_2 = -\pi/4$. In the case $\varphi_1 = \pi/2$ and $\varphi_2 = \pi/2$ we have the same figure as the left but with black circles. We used the meshes $N_1 = N_2 = 10$.

For the same parameters as those of the left in Fig. 1, the spin Chern number is, of course, $c_{\rm s} = 2 + 2 = 4$ in the limit $\gamma_1 = 0$. This spin Chern number remains unchanged for small but finite interlayer coupling γ_1. However, taking into account the gauge transformation $g(\varphi_i)$, the spin Chern number changes. In Fig. 3, we show examples of the n-field for $\gamma_1 = 0.1t$. We have the spin Chern numbers $2+2 = 4$, $2-2 = 0$, and $-2-2 = -4$: All of them are denoted as $c_{\rm s} = 0$ mod 4, which belong to the insulating phase. Detail analysis of this model including the interlayer coupling γ_3 will be published elsewhere.

Finally, we comment that the QSH effect is understood by the edge states [15], and therefore, it is interesting to establish the bulk-edge correspondence [27] for $\mathcal{T}$ invariant systems with respect to Z_2. We also mention that Fu and Kane [28] and Moore and Balents [29] have recently discussed the relationship between the Z_2 order and the spin Chern number, and reached a similar conclusion.

This work was supported in part by Grant-in-Aid for Scientific Research (Grant No. 17540347, No. 18540365) from JSPS and on Priority Areas (Grant No.18043007) from MEXT.

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